CLAIMS

1. A computer programmed to produce a three-dimensional representation of a molecule or molecular complex, wherein the molecule or molecular complex comprises a binding domain defined by the structure coordinates of

(a) Arg 39, His 110, Ser 132, Thr 136, Lys 254, Gly 297, Lys 311, Thr 315, Arg 337 and Asp 339 according to Fig. 1; or

(b) Ser 9, His 10, Arg 39, Asp 54, Arg 107, His 110, Ser 132, Ala 133, Arg 134, Thr 136, Arg 337 and Asp 339 according to Fig. 1,

or where the molecular complex or binding domain has a root mean square deviation of conserved residue backbone atoms of less than 2Å when superimposed on the relevant backbone atoms described by the structure coordinates of said amino acids.

2. A computer programmed according to claim 1, wherein (a) further comprises the structure coordinates of:

(i) Arg 45, Gly 109, Ala 111, Ser 131, Ala 133, Lys 238, Asp 240, Ile 250, Asn 251, Ala 252, Phe 253, Phe 294, Gly 296, Met 310, Ile 313, Pro 314, Ala 342, Ala 345, Ala 346 and Val 349 according to Fig. 1; or (b) further comprises the structure coordinates of:

(ii) Arg 45, Met 49, Asp 80, Ser 131, and Thr 137 according to Fig. 1,

or where the molecular complex or binding domain has a root mean square deviation of conserved residue backbone atoms of less than 2Å when superimposed on the relevant backbone atoms described by the structure coordinates of said amino acids, or where the molecular complex or binding domain has conservative amino acid substitutions for those amino acids specified in (i) or (ii).

3. A computer programmed according to claim 1 or claim 2, wherein (a further comprises the structure coordinates of Ser 338 according to Fig. 1, or (b) further comprises the structure coordinates of Arg 48, Glu 336 and Ser 338 according to Fig. 1.

4. A computer according to any of claims 1 to 3, wherein the molecule is Chorismate Synthase.

5. A computer according to any of claims 1 to 4, wherein the molecule is Chorismate Synthase from *S. pneumoniae*.

6. A method for identifying the potential of a chemical entity to associate with

Chorismate Synthase enzyme, comprising the steps of:

a) applying computational means to perform a fitting operation between the chemical entity and the Chorismate Synthase binding domain defined by the structure coordinates defined in any of claims 1 to 3; and

b) analysing the results of the fitting operation to quantify the association.

7. A method according to claim 6, wherein the computational means is provided by a computer as defined in any of claims 1 to 5.

8. A method for identifying a potential inhibitor or agent that interacts with a Chorismate Synthase binding domain, comprising the steps of:

(a) using the atomic coordinates defined in any of claims 1 to 3 to generate a three-dimensional structure of a molecule comprising a Chorismate Synthase binding domain;

b) employing the three-dimensional structure to design or select the inhibitor or agent;

c) synthesising the inhibitor or agent; and

d) contacting the inhibitor or agent with the Chorismate Synthase binding domain to determine the ability of the inhibitor or agent to interact with the domain.

9. A crystal of the binding domain of Chorismate Synthase, wherein the binding domain has a three-dimensional structure characterised by the atomic structure coordinates of Fig. 1.